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# Effect of structure and electronic property of chiral N, N′-dioxide-metal complexes on asymmetric catalysis: A theoretical study

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The $C_2$-symmetric chiral *N, N′*-dioxide-metal complexes developed by Feng's group have been proved to be kind of efficient and versatile catalysts for many asymmetric reactions, giving products in moderate to excellent yields and high enantioselectivities under mild conditions. Their catalytic performance including stereo-control inductive effect depended closely on the inherent properties of central metal ion such as Lewis acidity, ionic radius or coordination sphere properties as well as ligands' structures (amide substituent or the amino acid backbone). Herein, we selected four typical asymmetric reactions catalyzed by chiral *N, N′*-dioxide-metal complexes, that is, carbonyl-ene reaction, baeyer-villiger oxidation reaction, diels-alder reaction and friedel-crafts alkylation reaction to explore the corresponding reaction mechanisms by DFT and ONIOM methods. Furthermore, the structure and electronic property of metallic complexes formed by coordinating the chiral *N, N′*-dioxide ligands with different amino acid skeletons or straight-chain alkyl spacer (linkage) to different metal ions are studied. Our calculations revealed the characteristics of chiral environment and key structural subunits in ligands affecting the catalytic activities as well as chiral inductive effects. The inherent properties about metal-ligand cooperative catalysis as well as accommodation of substrate to catalyst's structure are also explored. Furthermore, the adjustment of counter ion on lewis acidity of metal center as well as donor-acceptor interaction between substrate and catalyst is also explored. These results are expected to suggest a model to predicated the likely stereo chemical outcome and provide useful information for rational design and synthesis of new chiral *N, N′*-dioxide-metal catalysts for asymmetric catalysis.

**Fig.1** The key factors affecting the stereo selectivity for reactions catalyzed by chiral *N, N′*-dioxide-metal complexes

## Recent publications

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5. Su Z S, Kim C K (2015) Trienamine catalysis for asymmetric diels–alder reactions of 2,4-dienones: A theoretical investigation. Organic and Biomolecular Chemistry 13:6313-6324.

## Biography

Zhishan Su is a Professor in College of Chemistry, Sichuan University (SCU). She studied Chemistry in SCU and received her PhD degree in Physical Chemistry under the supervision of Professor Changwei Hu in 2006. Between 2010 and 2012, she worked at the Inha University, Korea, as Assistant Professor and joined research group of Professor Chan Kyung Kim. She has been appointed as full Professor in 2015 in SCU and currently focuses on theoretical investigation on reaction mechanisms and design of new catalysts for asymmetric synthesis.

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